PhytoFit Userguide

2023-08-08 Stephanie.Clay@dfo-mpo.gc.ca

Authors

Chantelle Layton

Initial concept, preliminary design, coding, and algorithm development/improvements

Stephanie Clay

Final app design and modifications, feature addition, new datasets, maintenance, and algorithm improvements

Emmanuel Devred

Scientific support, algorithm development/improvements, review and feature recommendations

Acknowledgments

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How to cite

In publications, please include acknowledgments to **NASA OBPG** (https://oceancolor.gsfc.nasa.gov) for the raw satellite data and the **BIO remote sensing group** (https://github.com/BIO-RSG) for the application, and use this citation in the references:

Stephanie Clay, Chantelle Layton, & Emmanuel Devred. (2021). BIO-RSG/PhytoFit: First release (v1.0.0). Zenodo. https://doi.org/10.5281/zenodo.4770754

```
BibTeX format: @misc{clay21,
	author = {Clay, Stephanie and Layton, Chantelle and Devred, Emmanuel},
	title = "PhytoFit",
	howpublished = "\url{https://github.com/BIO-RSG/PhytoFit}",
	year = 2021
}
```

Prerequisites

- 1. Install the latest versions of R and RStudio.
- 2. Install the necessary packages:

```
install.packages(c("fst", "shiny", "shinyWidgets", "shinyjs", "shinybusy", "leaflet", "stars", "leafem", "leafpm"
, "quantreg", "minpack.lm", "sp", "ggplot2", "ggpp", "dplyr", "tidyr", "raster", "curl", "sf", "fs"))
remotes::install_github("BIO-RSG/oceancolouR")
# if the line above doesn't work, try devtools::install_github("BIO-RSG/oceancolouR")
# if that doesn't work, try either install.packages("remotes") or install.packages("devtools") and then run the o ceancolouR installation line again
```

3. Restart R after the packages have been installed.

Getting started

- 1. Download the PhytoFit repository (https://github.com/BIO-RSG/PhytoFit) one of two ways:
 - a. Option 1: Code --> Download ZIP
 - b. Option 2: Using git (this will make it easier to download updates in the future, by simply using the 'git pull' command):

Open git bash terminal, navigate to the folder where you want to download the repository, and type:

```
git clone https://github.com/BIO-RSG/PhytoFit.git
```

- 2. Open the PhytoFit repository in Rstudio (File --> Open Project --> Navigate to the PhytoFit folder and open PhytoFit.Rproj)
- 3. Download (or update) the datasets of your choice:

Open 00 download new datasets. R from the PhytoFit folder.

Set ask_user=FALSE to download all available datasets, or ask_user=TRUE to ask before downloading each one.

Alternatively, you can run the script from the command line like:

```
Rscript [script directory]/00 download new datasets.R 'false'
```

- * set "script directory" to the full path where the script is located
- * 'false' is the *ask_user* argument, set to 'true' for prompts

If you already have datasets in storage, you can update them using *OO_update_datasets.R*. Set the *ask_user* argument in the script and run from RStudio, or run from the command line (e.g. Rscript [script directory]/00 update datasets.R 'false').

4. Run the app by opening app.R in RStudio and clicking "Run app"

WARNINGS:

- Data files will be downloaded to data/[region]/ subfolders of the PhytoFit repository Do **NOT** move them from there or the app will not be able to read them.
- If possible, please keep the data files if you intend to use them in the future, rather than re-downloading them later, to avoid excessive traffic on the ftp server.
- Any data that is < 3 months old is "Near Real Time" (NRT) quality. NRT data is replaced with "Science quality" data after it becomes available, following the 3-month lag. More info here: https://lance.modaps.eosdis.nasa.gov/data/difference.php

Troubleshooting

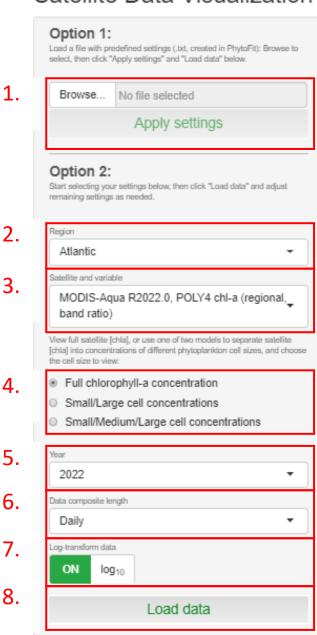
If you run into errors or the app crashes, try the following:

- Check if there are any helpful error messages in the console
- Clear memory: rm(list=ls())
- Restart R and/or RStudio
- Update packages used in the app

Main settings

- 1. If you have a settings file saved from a previous session, you can reapply it using this feature. **Warning: DO NOT EDIT THE SETTINGS FILE**, otherwise PhytoFit might not be able to read it properly.
- 2. Select your region and spatial resolution
 - Atlantic (42 to 71 °W, 39 to 63 °N)
 - Pacific (122 to 140 °W, 46 to 60 °N)
 - Gulf of Saint Lawrence (49 to 75 °W, 41 to 53 °N)
 - Baffin Bay (42 to 95 °W, 60 to 82 °N)
- 3. Select satellite and variable
 - Satellite sensors: MODIS-Agua, SeaWiFS, VIIRS-SNPP, OLCI-A or B
 - Variables: Chl-a (OCI, POLY4, GSM_GS, or EOF for the Gulf region only), SST (Sea Surface Temperature)
 - R20XX.X indicates the reprocessing (data version). More info here: https://oceancolor.gsfc.nasa.gov/data/reprocessing
- 4. Select Chl-a concentration type and cell size model (this is applied to Chl-a before logging, if selected)
- 5. Select year
- 6. Select temporal binning (daily data is averaged over composite period before logging, if selected)
- 7. Select logged or unlogged data
- 8. Load data for the current selection of settings

Satellite Data Visualization



Polygon selection

You can choose a polygon in order to calculate statistics and bloom metrics within that region. Click the "Polygon" button to expand this menu.

- 1. Choose a predefined polygon, or create your own.
- 2. For a custom polygon, optionally give it a name.
- 3. Select how you will define your custom polygon:
 - a) Draw using the controls at the top left corner of the map,
 - b) Type the coordinates, or
 - c) Select a shapefile containing a Simple Features object and click to select the polygon you want to use from the file.

Choose a polygon

Avalon Channel (AC)

AZMP

Avalon Channel (AC)

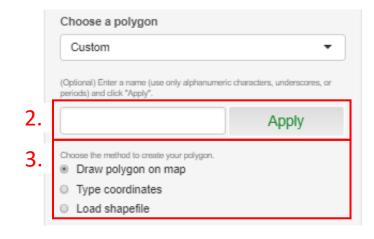
Central Labrador Sea (CLS)

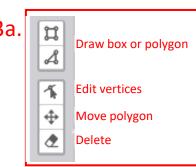
Cabot Strait (CS) V01

Cabot Strait (CS) V02

Central Scotian Shelf (CSS) V02

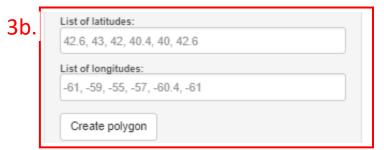
Eastern Scotian Shelf (ESS) V01



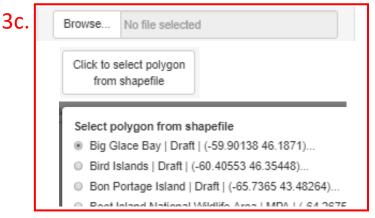


To close a polygon when you're done editing, click on the first point.

Only one polygon can be drawn on the map at a given time.



- Decimal degrees
- Separate coordinates by commas
- Use latitude/longitude < 0 for west/south

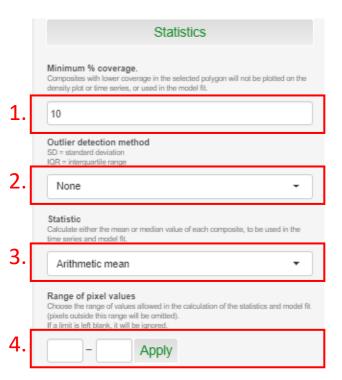


- Select the "shp" file and all files with the same name but different extensions (e.g. dbf, sbn, sbx, shx, prj, qix...)
- If the polygon has a large number of vertices, it might take several seconds to load.

Statistics

Click the "Statistics" button to expand this menu.

- 1. Select the minimum percent coverage required for a point in the time series to be used in the bloom fitting procedure or displayed in the density plot. If a daily (or 4-day, 8-day) composite has insufficient coverage within your polygon, it will be ignored.
- 2. Select the outlier detection method.
 - mean ± 2 standard deviations
 - mean ± 3 standard deviations
 - median ± 1.5 * interquartile range
 - Outer percentiles (0.01%, 0.1%, ...)
- 3. Select the statistic (mean or median) to use to summarize data within your polygon for each day (or 4-day or 8-day period).
- 4. To exclude data outside a certain range, enter the values here and click "apply". Data outside this range will not be included in the statistics or bloom fit. To ignore a boundary, leave it blank.



Model (bloom) fit

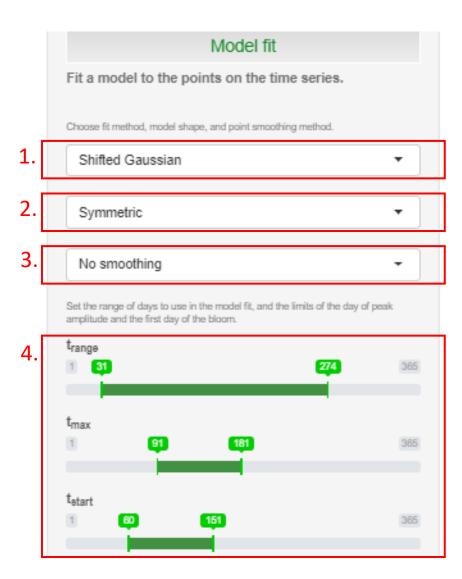
Click the "Model fit" button to expand this menu.

Each point in the time series and bloom fit is the daily (or 4-day, 8-day) spatial average (or median) of data after removal of outliers and points outside the desired range, using the binned data values. Only points with sufficient percent coverage inside the polygon on that day/week are used, within the range of days selected by the user.

- 1. Select the model to use in your fit. *Default = Shifted Gaussian*
- 2. Select the model shape around the bloom peak timing.
- 3. Choose whether to smooth points using LOESS locally estimated scatterplot smoothing) in the time series before fitting or just fit the raw data points. If you smooth the points, you must also set the "span", which controls the degree of smoothing:



4. Adjust the range of days to use in the fit, and restrict to a certain time window to search for the peak timing or start of the bloom period. t_{start} and t_{max} will be restricted based on t_{range} .



Model (bloom) fit (continued)

- 5. If you are modelling with a Shifted Gaussian, there are more options:
 - a) t_{start} calculation method
 - % amplitude: Define t_{start} as the day when the curve reaches a specified percentage of its amplitude over the background value, or
 - Constant threshold: Define t_{start} as the day when the curve reaches a specified threshold over the background value.
 - b) t_{max} switch

If this is ON, the bloom peak timing is allowed to vary as a parameter within the nonlinear least squares fitting procedure, rather than being a fixed value based on the actual maximum value.

WARNING: t_{start} can't be restricted if this is set to ON, because the t_{start} limits are set by restricting σ (the parameter controlling the width of the curve) relative to a known t_{max} value.

- c) Bt switch
 - If this is ON, the background line of the curve is allowed to vary linearly with time.
- d) weights
 - If this is ON, points in the fit are weighted by the percent coverage inside the polygon.
- e) Remove background
 - If this is checked, the background data line will be subtracted from the data points / curve before calculating the amplitude and magnitude.
- f) Fits are flagged (unaffected but marked) if the following occurs:
 - Flag 1: Flagged if amplitude_{fit}/ amplitude_{real} is outside the selected range
 - Flag 2: Flagged if magnitude_{fit} / magnitude_{real} is outside the selected range
 - Flag 3: Flagged if sigma <= temporal composite length (i.e. 1, 4, or 8 days)
 - Flag 4: Flagged if the calculated t_{start} is on the boundary of the t_{start} slider
 - Flag 5: Flagged if the calculated t_{max} is on the boundary of the t_{max} slider
 - Flag 6: Flagged if the calculated t_{end} is on the boundary of the t_{range} slider

You can adjust the range of acceptable ratio limits for flags 1 and 2 and click "apply".

6. If you are modelling with the Threshold method, set the threshold coefficient.

 t_{start} is defined as the point where chlorophyll-a drops below the threshold for > 14 days, measuring the days/weeks backward from the day of maximum concentration.

threshold = (threshold coefficient) * (median data value) median data value = median of all points used in bloom fit (within day range, with sufficient % coverage)

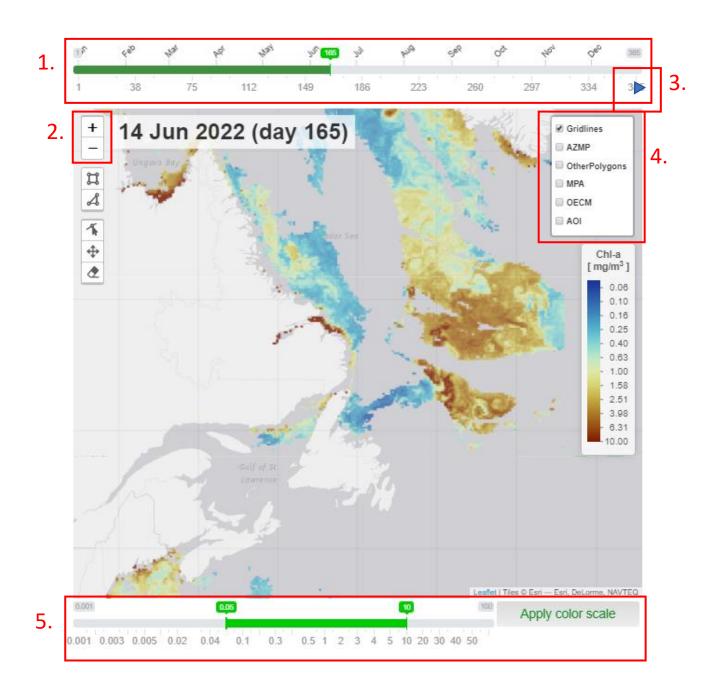


Threshold coefficient
The start of the phytoplankton bloom is considered to be the point before t_{exac} when [chla] drops below a threshold for > 14 days.
Threshold = chla_{median} * threshold coefficient

1.05

Output and display - Map

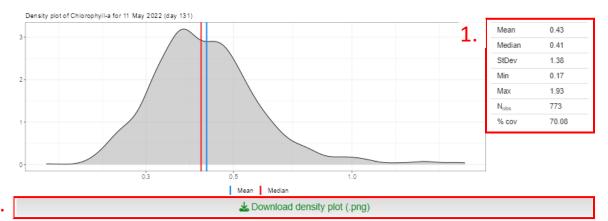
- 1. Day selector Move the slider to view the satellite imagery for that day (or 4-day or 8-day period)
- 2. Map zoom functions
- 3. Play button to allow map to load images in sequence with a 4-second delay between each image
- 4. Toggle groups of predefined polygons on the map, for viewing only
- 5. Adjust the color scale on the map



Output and display – Density plot

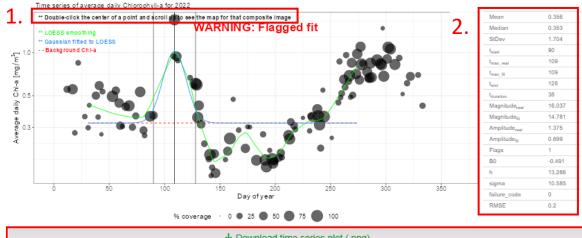
- 1. Daily (or 4-day, 8-day) statistics within your polygon
- 2. Click here to download this density plot with the table of statistics overlaid on the plot

2022 Atlantic, Avalon Channel (AC)



Output and display – Time series plot

- 1. Instruction to double-click the center of a point in the time series to load the satellite imagery and density plot for that point
- 2. Annual statistics, model parameters, and model metrics within your polygon
- 3. Download this time series plot with the table of stats and metrics overlaid
- Download a csv file containing the table of statistics within your polygon for each day (or 4-day, 8-day period) for the selected year
- 5. Download a table with the model parameters and metrics



3.	▲ Download time series plot (.png)				
4.	▲ Download time series table of statistics (.csv)				
5.	🚣 Download fit parameters (.csv)				

Model fits – Shifted Gaussian

$$B = B_0 + \beta t + \left(\frac{h}{\sqrt{2\pi}\sigma}\right) \exp\left(\frac{-(t - t_{max})^2}{2\sigma^2}\right)$$

 B_0 , β , h, and σ are calculated using nonlinear least squares. t_{max} is also calculated this way if the t_{max} switch is ON.

This is done with the *minpack.LM::nlsLM* function in R, which uses the Levenberg-Marquardt method. Starting guesses are required for the variables listed above (4 different sets of starting guesses are attempted during the fit), and lower/upper limits are enforced. If the curve is asymmetric, the same limits and guesses are used for each side. If the data is logged, B₀ limits and starting guesses are also logged.

If a Gaussian curve can't be fitted to the points, a failure code will be given in the output. These are the code meanings:

- Code 1: not enough data in the selected limits
- Code 2: nls failed
- Code 3: t_{start} threshold too high
- Code 4: t_{start} too early (before day 1)
- Code 5: t_{start} outside t_{range}
- Code 6: t_{end} outside t_{range}
- Code 7: data at end of bloom period is > threshold

Parameter	Units	Description	Lower limit	Upper limit	Starting guesses			
					1	2	3	4
В	mg.m ⁻³	Vector of data points in the time series						
t	Day of year	Vector of days, same length as B						
B_0	mg.m ⁻³	Background data value	0	5	0.5			
β (beta)	mg.m ⁻³ .day ⁻¹	Linear rate of change of B ₀	-0.02	0.01	-0.002	-0.002	0.001	0.001
h	Unitless	Controls the height of the curve	0	350	50	50	10	10
σ (sigma)	Unitless	Controls the width of the curve	0	100	10	2	2	1
t _{max}	Day of year	Day of maximum B	User-selected	User-selected	Day of maximum data value (within t _{max} limits)		_x limits)	

Model fits – Shifted Gaussian (continued)

$$B = B_0 + \beta t + \left(\frac{h}{\sqrt{2\pi}\sigma}\right) \exp\left(\frac{-(t - t_{max})^2}{2\sigma^2}\right)$$

Several metrics are collected, relating to the timing of the bloom and total data values. Some metrics are calculated using both the Gaussian curve and the real data points.

Metric	Units	Description
t _{start}	Day	Start of the bloom
t _{max_real}	Day	Timing of maximum value within bloom period
t _{max_fit}	Day	Timing of peak of Gaussian curve
t _{end}	Day	End of the bloom
t _{duration}	Day	Duration of the bloom
Amplitude _{real}	mg.m ⁻³	Maximum value within bloom period
Magnitude _{real}	mg.m ⁻³ .day	Area under the real data points within the bloom period
Amplitude _{fit}	mg.m ⁻³	Peak of Gaussian curve
Magnitude _{fit}	mg.m ⁻³ .day	Area under the Gaussian curve within the bloom period

- If "remove background" has been checked, the background data will be subtracted before calculating amplitude and magnitude.
- If points between t_{start} and t_{end} are below the background line and "remove background" has been selected, the magnitude (area) below the line will be negative so it will be subtracted from the final value (this only affects Magnitude_{real}).
- If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points. The curve is then fit to the LOESS values. Note that in this case, the mean, median, Amplitude_{real}, and Magnitude_{real} are still calculated using the real data values.

Model fits – Rate of Change

This algorithm does not model a curve like the Shifted Gaussian, but only calculates the maximum, start, and end days of the bloom.

The maximum is selected as the day of actual maximum concentration, within the selected range.

The initiation is the day of the maximum rate of change in concentration, within the selected bounds.

If any indices cannot be computed, they will be blank and not appear on the time series plot. This might happen due to an insufficient number of data points in the time series, or within the range of days allowed for the start or day of maximum concentration of the bloom.

B₀ (the background data value) is computed using the R function *quantreg::rq* to perform a quantile regression (25th percentile) on the full dataset (days/weeks with sufficient percent coverage), and is subtracted from the data to calculate the final amplitude and magnitude metrics.

Metric	Units	Description
t _{start}	Day	Start of the bloom
t _{max_real}	Day	Timing of maximum value within bloom period
t _{end}	Day	End of the bloom
t _{duration}	Day	Duration of the bloom
Amplitude _{real}	mg.m ⁻³	Maximum value within bloom period
Magnitude _{real}	mg.m ⁻³ .day	Area under the real data points within the bloom period

• If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points.

Model fits - Threshold

This model is similar to the Rate of Change:

- It only calculates the maximum, start, and end days of the bloom
- B₀ is calculated using *quantreg::rq* and subtracted from the data points to get amplitude and magnitude
- The maximum is selected as the day of actual maximum concentration, within the selected range.

The initiation is defined as the day the data drops below a threshold for > 14 consecutive days, working backward from the day of the maximum value.

If your data are not logged:

Threshold = (Threshold coefficient) * (median data used in the fit)

If your data are logged:

Threshold = log10 [(Threshold coefficient) * 10^{(median log10(data) used in the fit)}]

Threshold coefficient = user-selected

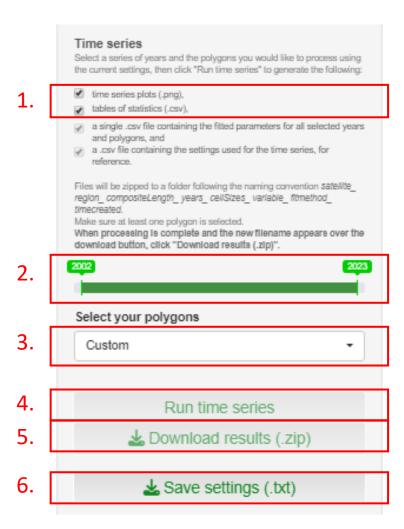
Metric	Units	Description
t _{start}	Day	Start of the bloom
t _{max_real}	Day	Timing of maximum value within bloom period
t _{end}	Day	End of the bloom
t _{duration}	Day	Duration of the bloom
Amplitude _{real}	mg.m ⁻³	Maximum value within bloom period
Magnitude _{real}	mg.m ⁻³ .day	Area under the real data points within the bloom period

 If LOESS smoothing and point-weighting are both selected, the LOESS-smoothed curve will be calculated using the weighted real data points.

Run full time series and save settings

At the bottom of the left panel, you have the option of collecting statistics and fitting the model for multiple years of data, and downloading the collection of results in a zip file.

- 1. Check these boxes if you want to include the time series plots in png format in the output, and the table of statistics in csv format.
- 2. Adjust the slider to the range of years you want to process.
- 3. Select the polygons you want to use in the processing.
- 4. Click "Run time series" to run the calculations, then
- 5. Click "Download results" to download the zip file, which uses the following naming convention: satellite_region_compositeLength_years_cellSizes_variable_fitmethod_timecreated
- 6. Save a settings file for the current selection of settings.



AZMP fitting parameters

Annual reporting for the AZMP (Atlantic Zone Monitoring Program, https://www.dfo-mpo.gc.ca/science/data-donnees/azmp-pmza/index-eng.html) includes statistics and bloom metrics for a set of polygons. Previously, AZMP boxes were typically fitted using a Fortran script, examining and adjusting every fit manually. Results were stored here: https://ftp.dfo-mpo.gc.ca/bometrics/spring-bloom. Below are the settings to use in PhytoFit to most closely replicate these fitting procedures. Unavoidable differences between the original procedure and PhytoFit are highlighted in red.

L2 and L3 flag info here: https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags

	Original Fortran bloom fitting system	PhytoFit bloom fitting
Sensor	VIIRS-SNPP	VIIRS-SNPP
Spatial resolution	~1km	4km
Projection	Equidistant cylindrical	Binned
Level-2 flags	All L2 flags except TURBIDW	L3 flags + FILTER
Chl-a model	OCI, not logged	OCI, not logged
Temporal binning	Weekly (using a 4-week-per-month system)	8-day
Minimum % coverage	1%	1%
Outliers	Not removed	Not removed
Statistic	Average	Average
Range of pixel values	<= 64 mg.m ⁻³	<= 64 mg.m ⁻³
Model	Symmetric Shifted Gaussian No smoothing, no point weighting, flat background (i.e. beta OFF), t_{max} defined as day of max concentration (i.e. t_{max} switch OFF)	Symmetric Shifted Gaussian No smoothing, no point weighting, flat background (i.e. beta OFF) , t_{max} defined as day of max concentration (i.e. t_{max} switch OFF)
Range of days used in fit	Feb-July, or Feb-Aug for boxes >= 56°N	t _{range} 31-212 (boxes < 56°N), 31-244 (boxes >= 56°N)
Gaussian fit flags	Box has <10% coverage, flags 1-3 listed in PhytoFit	[See 6 flags listed in Shifted Gaussian description]
t _{start} calculation	20% curve amplitude	20% curve amplitude
Bloom metrics	Remove background before calculating amplitude, magnitude	Remove background before calculating amplitude, magnitude

Extra tools

In the tools subfolder of the repository, there are a few extra R scripts:

Scripts to create your own region and predefined polygons:

- tools_01a_define_polygons.R
- tools 01b create new region.R

Scripts to concatenate and format the output from PhytoFit:

- tools_02_format_bloommetrics.R
- · tools fit bloom from chla.R

This standalone script can accept a dataframe with year, doy, and chl columns, and fit a bloom to the chl using the same settings as used in the app.

This is useful for fitting blooms to in situ data records that only have one value per day or week.

To use this script on your own computer, you must also download `functions.R`, `gaussFit.R`, `threshold.R`, and `rateOfChange.R`.

Required packages: `dplyr`, `oceancolouR`*, `minpack.lm`

Optional packages for plotting results: 'ggplot2', 'patchwork'

*The oceancolouR package, which can be installed with one of the following commands in R:

```
remotes::install_github("BIO-RSG/oceancolouR", build_vignettes = TRUE)
devtools::install_github("BIO-RSG/oceancolouR", build_vignettes = TRUE)
```

References and data sources

Bloom fitting models (Shifted Gaussian, Rate of Change, and Threshold methods) :

TECH REPORT IN PROGRESS

• Chlorophyll-a algorithm **OCx**:

O'Reilly, John & Maritorena, S. & Mitchell, B.G. & Siegel, David & Carder, Kendall & Garver, S.A. & Kahru, Mati & Mcclain, Charles. (1998). Ocean color chlorophyll algorithms for SeaWiFS. Journal of Geophysical Research. 103. 937-953.

https://www.researchgate.net/publication/284463756 Ocean color chlorophyll algorithms for SeaWiFS

Chlorophyll-a algorithm GSM:

Maritorena, Stéphane & Siegel, David & Peterson, Alan. (2002). Optimization of a semianalytical ocean color model for global-scale application. Applied optics. 41. 2705-14. 10.1364/AO.41.002705.

https://www.researchgate.net/publication/11345370 Optimization of a semianalytical ocean color model for global-scale application

Chlorophyll-a algorithms OCx, POLY4, and GSM GS (regional tuning):

Clay, S.; Peña, A.; DeTracey, B.; Devred, E. Evaluation of Satellite-Based Algorithms to Retrieve Chlorophyll-a Concentration in the Canadian Atlantic and Pacific Oceans. Remote Sens. 2019, 11, 2609.

https://www.mdpi.com/2072-4292/11/22/2609

• Chlorophyll-a algorithm **EOF**:

Laliberté, J.; Larouche, P.; Devred, E.; Craig, S. Chlorophyll-a Concentration Retrieval in the Optically Complex Waters of the St. Lawrence Estuary and Gulf Using Principal Component Analysis. Remote Sens. 2018, 10, 265.

https://www.mdpi.com/2072-4292/10/2/265

References and data sources (continued)

Phytoplankton cell size model 1 (small/large cells):

Devred, Emmanuel & Sathyendranath, S & Stuart, V & Maass, H & Ulloa, Osvaldo & Platt, T. (2006). A two-component model of phytoplankton absorption in the open ocean: Theory and applications. Journal of Geophysical Research. 111. 10.1029/2005JC002880.

https://www.researchgate.net/publication/229086123 A two-component model of phytoplankton absorption in the open ocean Theory and applications

Phytoplankton cell size model 2 (small/medium/large cells):

Devred, Emmanuel & Sathyendranath, Shubha & Stuart, Venetia & Platt, Trevor. (2011). A three component classification of phytoplankton absorption spectra: Application to ocean-color data. Remote Sensing of Environment - REMOTE SENS ENVIRON. 115. 2255-2266. 10.1016/j.rse.2011.04.025.

https://www.researchgate.net/publication/251494326 A three component classification of phytoplankton absorption spectra Application to ocean-color data

Phytoplankton cell size models (updated coefficients):

Liu, Xiaohan & Devred, Emmanuel & Johnson, Catherine. (2018). Remote Sensing of Phytoplankton Size Class in Northwest Atlantic from 1998 to 2016: Bio-Optical Algorithms Comparison and Application. Remote Sensing. 10. 10.3390/rs10071028.

https://www.researchgate.net/publication/326033452 Remote Sensing of Phytoplankton Size Class in Northwest Atlantic from 1998 to 2016 Bio-Optical Algorithms Comparison and Application#pf18

Raw data:

Daily level-3 binned files are downloaded from NASA OBPG (https://oceancolor.gsfc.nasa.gov), and weekly composites are generated by taking a simple arithmetic average of each pixel over the selected composite period (e.g. 4 days or 8 days). The binned data is used for statistics and bloom fitting, projected onto a regular grid on the map for display.

- NASA OCI chlorophyll-a algorithm: https://oceancolor.gsfc.nasa.gov/resources/atbd/chlor_a
- Level-3 binned files: https://oceancolor.gsfc.nasa.gov/l3
- Binning scheme: https://oceancolor.gsfc.nasa.gov/resources/docs/format/l3bins
- Level-2 and 3 default flags: https://oceancolor.gsfc.nasa.gov/resources/atbd/ocl2flags
 (PhytoFit data uses these default flags + FILTER flag)